SUPPORTING INFORMATION

Finding Correlations of the Oxygen Reduction Reaction Activity of Transition Metal Catalysts with Parameters Obtained from Quantum Mechanics

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Table S1. Lattice parameters (Å) used for bulk and surface calculations.

Metal	Fe	Co	Ni	Cu	Ru	Rh	Pd	Ag	Os	Ir	Pt	Au
Lattice Parameter	2.87	2.50	3.52	3.61	2.71	3.80	3.89	4.09	2.73	3.84	3.92	4.08

For Fe, the parameter is the cubic edge length of BCC. For Co, Ru, and Os, the parameter is length "a" of HCP. For Ni, Cu, Rh, Pd, Ag, Ir, Pt, and Au, the parameter is the cubic edge length for FCC.

Table S2. The most favorable binding sites for pure metals.

Metal / BE	Fe	Co	Ni	Cu	Ru	Rh	Pd	Ag	Os	Ir	Pt	Au
H	2a	3h	3f	3h	3f	3f	3f	3f	3f	1	1	3f
HOH	1	1	1	1	1	1	1	1	1	1	1	1
O	2a	3f	3f	3f	3h	3f	3f	3f	3h	3f	3f	3f
OH	2a	3h	3f	3f	3f	2t	2t	3f	3h	2t	3h	2t
OO	3	3h	2t	3h	3f	3h	3f	2t	3h	2b	3f	3f
OOH	1	1	1	1	1	1	1	1	1	1	1	1

BCC (110): Fe

1: 1-fold position.

2a: 2-fold position between lying on the cubic lattice edge (2.87 Å)

3: 3-fold position.

FCC (111): Ni, Cu, Rh, Pd, Ag, Ir, Pt, Au HCP (0001): Co, Ru, Os

1: 1-fold position.

2t: 2-fold position lying directly on top.

2b: 2-fold position slightly bends in the direction of a CCP position.

3f: 3-fold position lying over FCC site.

3h: 3-fold position lying over HCP site.

Table S3. OH binding energy (eV) on the (100) surface for listed metals and the most favorable binding position.

Metal	Ni	Cu	Rh	Pd	Ag	Ir	Pt	Au
Binding Energy	3.50	3.15	3.12	3.69	2.74	2.96	2.87	2.20
Binding Site	2-fold	2-fold	2-fold	2-fold	4-fold	2-fold	2-fold	2-fold

Table S4. Calculated NEB barriers (eV) of the ORR surface reactions for the Pt (100) surface. The RDS is H_2O formation with a barrier of 0.52 eV, higher than that for the Pt (111) surface (0.28 eV)

Reaction step	Barrier
O_2 Dissociation: $O_{2a} \rightarrow 2O_a$	0.10
OOH Formation: $O_2 + H_a \rightarrow OOH_a$	0.17
OOH Dissociation: $OOH_a \rightarrow O_a + OH_a$	0
OH Formation: $O_a + H_a \rightarrow OH_a$	0.30
O Hydration: $O_a + H_2O_a \rightarrow 2OH_a$	0
H_2O Formation: $OH_a + H_a \rightarrow H_2O_a$	0.52
RDS	0.52

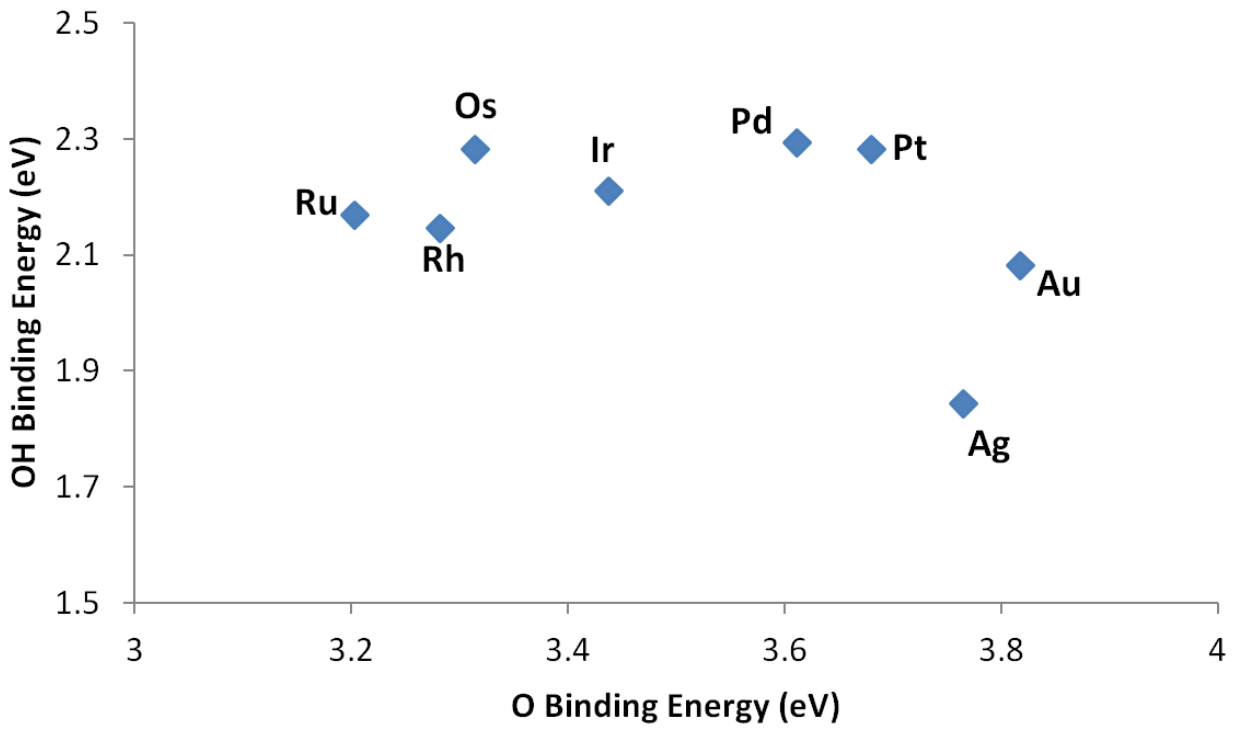

Figure S1. Calculated O and OH binding energy of Pt-monolayer/metal catalysts.
The observed relationship is not linear. The labeled atom is the substrate and a single layer of Pt sits on top. The binding geometry for OH is a 3-fold HCP position and for O is a 3-fold FCC position.